

First Order Phase Transition and Phase Coexistence in a Spin-Glass Model

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We study the mean-field static solution of the Blume-Emery-Griffiths-Capel model with quenched disorder, an Ising-spin lattice gas with quenched random magnetic interaction. The thermodynamics is worked out in the Full Replica Symmetry Breaking scheme. The model exhibits a high temperature/low density paramagnetic phase. When the temperature is decreased or the density increased, the system undergoes a phase transition to a Full Replica Symmetry Breaking spin-glass phase. The nature of the transition can be either of the second order (like in the Sherrington-Kirkpatrick model) or, at temperature below a given critical value (tricritical point), of the first order in the Ehrenfest sense, with a discontinuous jump of the order parameter and a latent heat. In this last case coexistence of phases occurs.

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The spin-glass phase (SG) has played and is still playing a central role in the understanding of disordered and complex systems. The analysis of mean-field models revealed different possible scenarios for the SG phase and the transition to it. Most of the work, however, has been concentrated on just two of them. In order of appearance in literature the first scenario is described by a Full Replica Symmetry Breaking (FRSB) solution characterized by a continuous order parameter function [1], which continuously grows from zero by crossing the transition. The prototype model is the Sherrington-Kirkpatrick (SK) model [2], a fully connected Ising-spin with quenched random magnetic interactions. The second scenario, initially introduced by Derrida [3], provides a transition with a jump in the order parameter to a SG One Step Replica Symmetry Breaking (1RSB). No discontinuity appear, however, in the thermodynamic functions. Actually, at the transition to the 1RSB SG phase the Edwards-Anderson order parameter can either grow continuously from zero or jump discontinuously to a finite value. The first case includes Potts-glasses with three or four states [4], the spherical p -spin spin glass model in strong magnetic field [5] and some spherical p -spin spin glass model with a mixture of $p = 2$ and $p > 3$ interactions [6, 7]. The latter case includes, instead, Potts-glasses with more than four states [4], quadrupolar glass models [4, 8], p -spin interaction spin-glass models with $p > 2$ [3, 9, 10] and the spherical p -spin spin glass model in weak magnetic field [5]. The models of this class, often referred to as “discontinuous spin glasses” [11], have been widely investigated in the last years because of their relevance for the structural glass transition observed in fragile glasses [10, 12].

In all cases discussed so far the transition is *always* continuous in the Ehrenfest sense. To our knowledge, the first case of a spin glass undergoing a genuine first order thermodynamic transition is the so called Ghatak-Sherrington model (GS) [13]. However, besides the full

analysis of the RS solution, the study of the FRSB solution for this model was done only close to the continuous transition (SK-like) down to and including the tricritical point because of its complexity [13, 14]. We also recall that an exactly solvable model, generalization of the Derrida’s REM [3], displaying a first order phase transition to a SG phase with latent heat, was introduced by Mottrishaw [15]. However, at difference with the GS model, the SG phase is 1RSB.

Recently a generalization of the GS model [13] has been considered in connection with the structural glass transition due to the conjectured existence [16] of a “discontinuous”, in the above mentioned sense, transition to a 1RSB SG phase. This possibility has risen new interest in such model and its finite dimensions version has been numerically investigated in a search for evidence of a structural glass transition scenario [17].

To clarify this issue and its compatibility with previous results on the GS model, we have investigated the whole phase diagram, deep in the SG phase, for the mean field quenched disorder variant of the Blume-Emery-Griffiths-Capel model [18] (BEGC), introduced for the λ transition in mixtures of He^3 - He^4 , which includes the GS model.

In literature there exists two different versions of the model. The first one is the direct generalization of the original BEGC model and uses spin-1 variables $\sigma_i = -1, 0, 1$ on each site i of a lattice [19, 20], while the second formulation is a lattice gas ($n_i = 0, 1$) of spin-1/2 variables ($S_i = -1, 1$) [16, 21]. In both cases the spin variables interact through quenched random couplings. The two formulations are equivalent, at least as far as static properties are concerned. Indeed, by imposing $\sigma_i \equiv S_i n_i$ the two models can be transformed one into the other, apart from a rescaling of the chemical potential/crystal field [22]. In this paper we will use the second formulation

described by the Hamiltonian (DBEGC) [16]

$$\mathcal{H} = - \sum_{i < j} J_{ij} S_i S_j n_i n_j - \frac{K}{N} \sum_{i < j} n_i n_j - \mu \sum_i n_i \quad (1)$$

representing an Ising spin glass lattice gas coupled to a spin reservoir. The symmetric couplings J_{ij} are quenched Gaussian random variables of zero mean and variance $\overline{J_{ij}^2} = \overline{J_{ji}^2} = J^2/N$. Here and in the following the overline denotes average with respect to disorder. Limiting cases of the model are the SK model [2] obtained for $\mu/J \rightarrow \infty$, the site frustrated percolation model [23] for $K = -1$ and $J/\mu \rightarrow \infty$, and the GS model for $K = 0$.

To keep the level of the presentation as general as possible, we shall avoid technical details and report only the main results for the phase diagrams for the three relevant cases of the GS model ($K = 0$), the frustrated Ising lattice gas ($K = -1$) and the case of attracting particle-particle interaction ($K = 1$).

Applying the standard replica method, the FRSB solution in the SG phase is described by the order parameter function [1]

$$q(x) = \int_{-\infty}^{\infty} dy P(x, y) m(x, y)^2, \quad (2)$$

and the density of occupied sites by

$$\rho = \int_{-\infty}^{\infty} dy P(1, y) \frac{\cosh \beta J y}{e^{-\Theta_1} + \cosh \beta J y}, \quad (3)$$

where $\Theta_1 \equiv (\beta J)^2 [\rho - q(1)]/2 + \beta(\mu + K\rho)$ and $m(x, y)$ and $P(x, y)$ [24] are solution of

$$\dot{m}(x, y) = -\frac{\dot{q}}{2} m''(x, y) + \dot{\Delta}(x) m(x, y) m'(x, y), \quad (4)$$

$$\dot{P}(x, y) = \frac{\dot{q}(x)}{2} P''(x, y) + \dot{\Delta}(x) [P(x, y) m(x, y)]', \quad (5)$$

with boundary conditions

$$m(1, y) = \frac{\sinh(\beta y)}{e^{-\Theta_1} + \cosh(\beta y)}, \quad (6)$$

$$P(0, y) = \frac{1}{\sqrt{2\pi q(0)}} \exp \left\{ -\frac{y^2}{2q(0)} \right\}. \quad (7)$$

The functions $m(x, y)$ and $P(x, y)$ are, respectively, the local magnetization and local field probability distribution at “time scale” $x \in [0, 1]$ [24], while $\Delta(x)$ is the Sompolinsky’s anomaly [25]. As usual, the “dot” denotes partial derivative with respect to x while the “prime” the one with respect to y .

All thermodynamic quantities can be written in terms of the above functions. For example, defining $\tilde{K} \equiv K + \beta J/2$, the internal energy density u and the entropy density s read

$$u = -\frac{\tilde{K}}{2} \rho^2 - \mu \rho + \frac{\beta J^2}{2} q(1)^2 + \int_0^1 dx q(x) \dot{\Delta}(x), \quad (8)$$

$$\begin{aligned} s = & -\rho \Theta_1 - \frac{(\beta J)^2}{4} [\rho - q(1)]^2 + \int_{-\infty}^{\infty} dy P(1, y) \\ & \times \{ \log [2 + 2 e^{\Theta_1} \cosh(\beta J y)] - \beta J y m(1, y) \} \end{aligned} \quad (9)$$

We have solved the coupled equations (2)-(5) in the Parisi’s gauge $\dot{\Delta} = -\beta J x \dot{q}(x)$ using the pseudo-spectral method introduced in [26]. Analyzing the stability of the RS solution one gets the critical lines

$$1 - (\beta J \rho)^2 = 0, \quad (10)$$

$$1 - \beta \tilde{K}(1 - \rho) \rho = 0, \quad (11)$$

above which the only solution is the paramagnetic (PM) solution $q(x) \equiv 0$ for $x \in [0, 1]$, $\rho = 1/[1 + e^{-\Theta_1}]$. This is stable for any value of K . In the $T - \rho$ plane, these are, respectively, the straight line and the left branch of the spinodal line shown, in Figs. 1, 6 and 8 (for $K = 1, 0, -1$, respectively). The two lines meet at the tricritical point

$$T_c = \rho_c = \frac{-3/2 + K + \sqrt{K^2 - K + 9/4}}{2K}, \quad (12)$$

$$\mu_c = -\frac{1}{2} - \rho_c \left[K + \log \left(\frac{1}{\rho_c} - 1 \right) \right]. \quad (13)$$

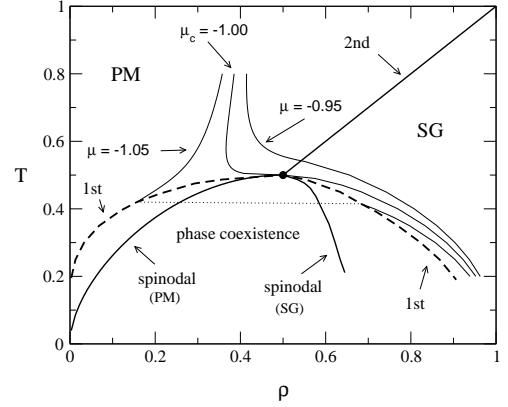


FIG. 1: $T - \rho$ phase diagram of the DBEGC for $K = 1$. The dot marks the tricritical point $\mu_c = -1$, $T_c = 1/2$, $\rho_c = 1/2$. See text for discussion.

By crossing the critical line (10) above the tricritical point ($\rho > \rho_c$, $T > T_c$, $\mu > \mu_c$) the system undergoes a continuous phase transition of the SK-type to a FRSB SG phase, with a non-trivial continuous order parameter function $q(x)$ which smoothly grows from zero.

Below the tricritical point the scenario is completely different with a transition from the PM phase to a FRSB SG phase with $q(x)$ which discontinuously jumps from zero to a non-trivial (continuous) function. At the critical temperature the entropy is discontinuous, see Fig. 2, and hence a latent heat is involved in the transformation, implying that the transition is of the first order in the Ehrenfest sense. The transition line is determined by the free energy balance between the PM and the SG

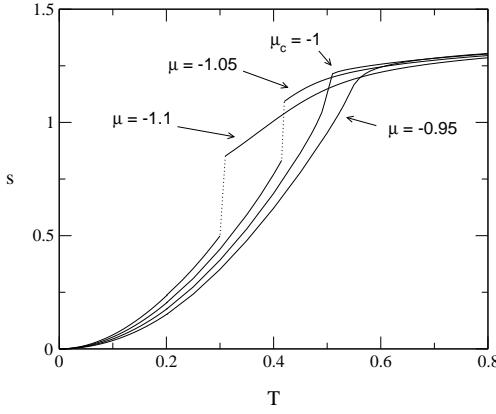


FIG. 2: Entropy density as a function of temperature for $K = 1$. For $\mu < \mu_c = -1$ the entropy is discontinuous at the transition temperature.

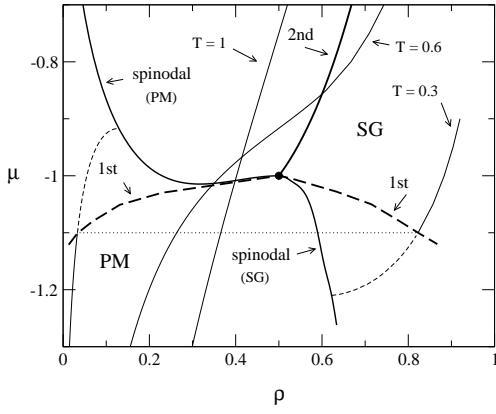


FIG. 3: $\mu - \rho$ phase diagram of the DBEGC for $K = 1$. Three isothermal lines are plotted, two above and one below the tricritical temperature $T_c = 1/2$. For $T = 0.3$ also the metastable branches are shown, both in the RS PM phase and in the FRSB SG phase. They reach the spinodal lines with zero derivative. In this plane of conjugated thermodynamic variables a Maxwell construction can be explicitly performed.

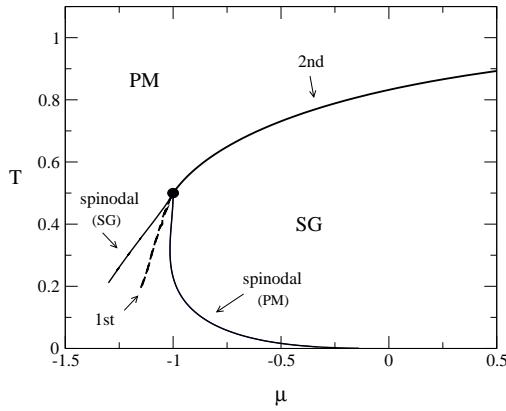


FIG. 4: $T - \mu$ phase diagram of the DBEGC for $K = 1$.

phase [15], and is shown as a broken line in the phase diagrams. The line (11) where the PM solution becomes unstable, and the equivalent line from the SG side are the *spinodal* lines. This can be better appreciated in the $\mu - \rho$ plane. From Fig. 3 we indeed see that the isother-

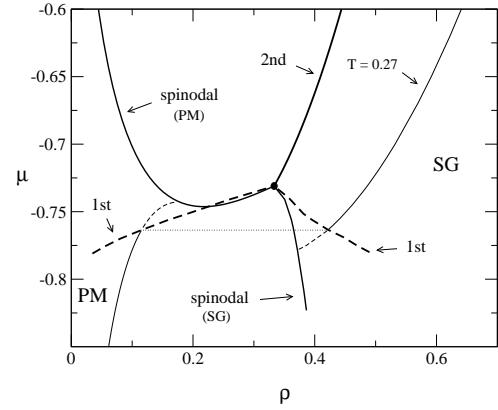


FIG. 5: $\mu - \rho$ phase diagram of the DBEGC for $K = 0$. The dot marks the tricritical point $\mu_c = -0.731$, $T_c = 1/3$, $\rho_c = 1/3$. The isothermal at $T = 0.27$ is plotted, together with its metastable parts (dotted line) both in the SG and in the PM phase.

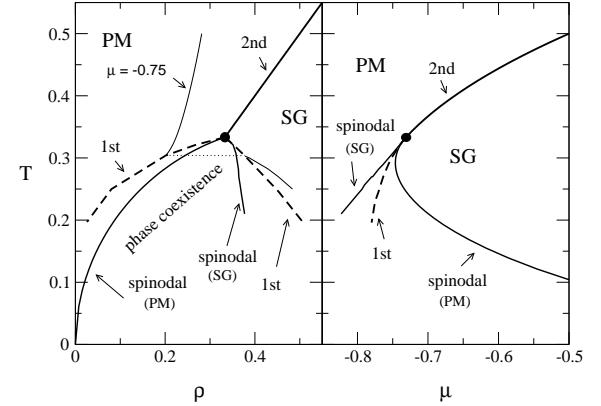


FIG. 6: $T - \rho$ and $T - \mu$ phase diagrams for $K = 0$. A line at constant $\mu = -0.75 < \mu_c$ is shown in the $T - \rho$ plane.

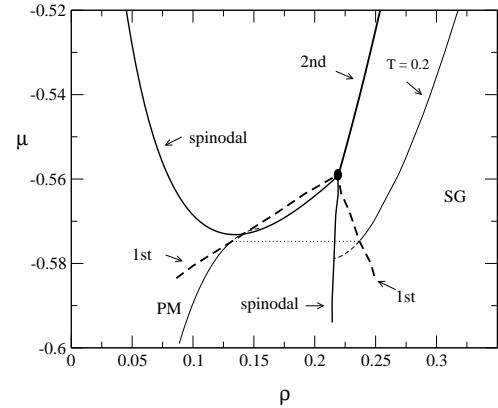


FIG. 7: $\mu - \rho$ phase diagram of the DBEGC for $K = -1$, with isothermal at $T = 0.2 < T_c$. The dot marks the tricritical point $\mu_c = -0.559$, $T_c = 0.219$, $\rho_c = 0.219$.

mal lines cross the instability lines with zero derivative and hence a diverging compressibility $\kappa = (1/\rho^2)\partial\rho/\partial\mu$. It can be shown that the first order transition line can be determined in the $\mu - \rho$ phase diagram from the isothermal and spinodal lines by using a Maxwell construction. In the region between the first order transition line and

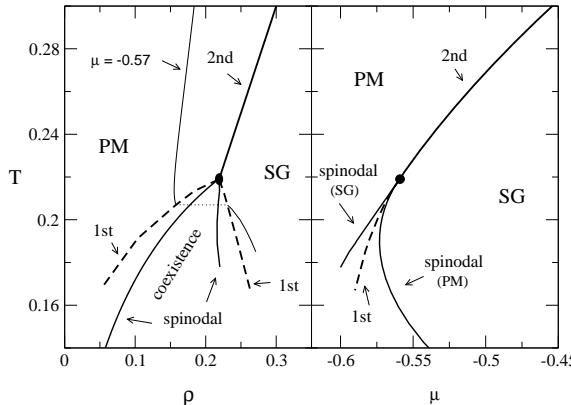


FIG. 8: $T - \rho$ and $T - \mu$ phase diagrams for $K = -1$. In the $T - \rho$ plane the line at constant $\mu = -0.57 < \mu_c$ is plotted.

the spinodal line the pure phase is metastable. Below the spinodal lines (in the $T - \rho$ plane) no pure phase can exist and the system is in a mixture of PM and SG phase (*phase coexistence*). Finally, the phase diagram in the $T - \mu$ plane, for $K = 1$, is shown in Fig. 4.

By varying K the scenario remains qualitatively unchanged. The only effect of a strong repulsive particle-particle interaction is to increase the phase diagram zone where the empty system ($\rho = 0$) is the only stable solution. In order to find further phases, e.g. an anti-quadrupolar phase [16], a generalization of the present analysis to a two component magnetic model [27], including quenched disorder, has to be carried out [28]. In Figs. 6-7 we show the phase diagrams for $K = 0$, the GS model [13], and $K = -1$ the frustrated lattice gas [17].

In conclusion, we have discussed the complete phase diagram of the DBEGC model in the mean field limit, explicitly solving the FRSB equations in the whole SG phase with the pseudo-spectral method developed in Ref. [26]. Our results rule out the possibility of a 1RSB phase: the SG phase is *always* of FRSB type. The transition between the PM phase and the SG phase can be either of the SK-type or, below the tricritical temperature, a first order thermodynamic phase transition. In the latter case, like in the gas-liquid transition, a latent heat is involved in the transformation. Moreover, for a certain range of parameters (between the spinodal lines), no pure phase is achievable, not even as a metastable one, and the two phases coexist.

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